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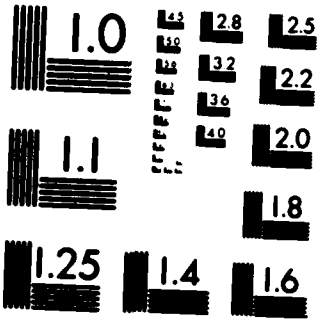

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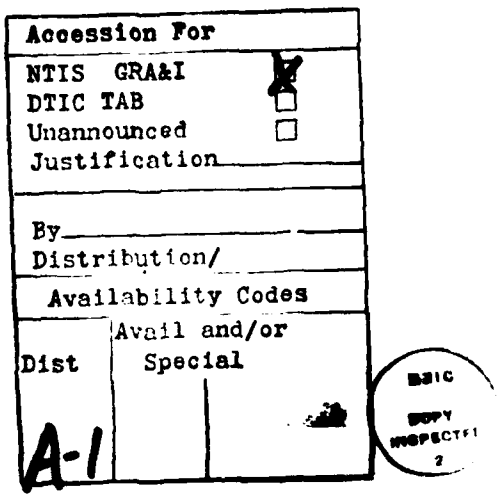

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THERMODYNAMIC EXTRAPOLUTION OF ROCKET ENGINE PERFORMANCE PARAMETERS

Ge Minglong

Abstract

This paper uses one isentropic reference line and two isenthalpic partial derivatives to establish extrapolation formulas of rocket engine performance parameters. These formulas can be used for the extrapolation calculations of specific thrust, characteristic velocity, nozzle-area ratio and the thermodynamic parameters at the combustion chamber and the nozzle exit when there are changes in the initial enthalpy of the propellant, combustion chamber pressure and nozzle exit pressure.

I. Preface

The thermodynamic calculation method for rocket engine ideal performance is classic. It has been introduced in Reference 1 and other books and periodicals on rocket engines. This diverse calculation is very useful for the design of rocket engines yet the time expended is relatively great and it is not convenient to arrange and put into book form the large amount of data. Therefore, the problem of the extrapolation calculation of the rocket engine's theoretical performance parameters was brought forth early. Many people have given formulas for thermodynamic extrapolation calculation [2-5].

In recent years, following the popularization of pocket electronic calculators, the use of the extrapolation calculation method to determine the ideal performance of rocket engines is even more convenient. For this reason, on the basis of existing extrapolation formulas, this paper derives even more

accurate extrapolation formulas.

II. Isentropic Reference Lines

Because of the element compositions of certain propellants made up of mixed ratio O/F of determined value are fixed, regardless of the propellant's initial enthalpic value which is affected by the environmental temperature and other factors being Ho numerical value (H_{co} or H_c) and no matter how large the combustion chamber pressure (p_{co}, p_c, or p_c) is and how large the nozzle exit pressure (p_{co}, p_c', p_c'' or p_c), the ideal thermodynamic process of the rocket engine and isentropic limited balance expansion process can be expressed as the different isentropic lines $c_o t_o e_o e''$... etc. on the same enthalpy-entropy chart as shown in Fig. 1.

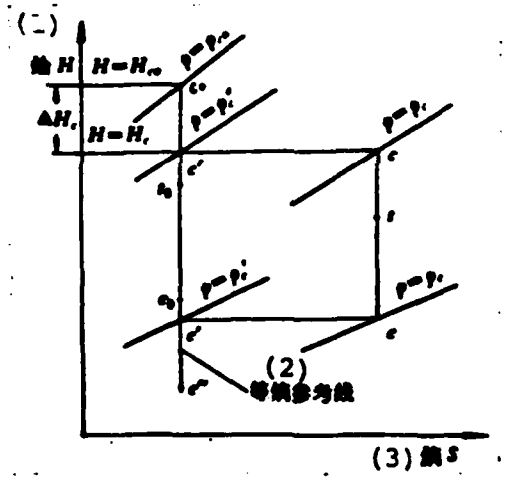

Fig. 1 Enthalpy-entropy schematic diagram.
Key: (1) Enthalpy; (2) Isentropic reference line; (3) Entropy.

By carrying out accurate thermodynamic calculations of a given propellant's initial enthalpic value (H_{co}) and combustion chamber pressure (p_{co}), we can determine the thermodynamic parameters of combustion chamber state point c_o and throat state point t_o. Afterwards, we selected a certain nozzle exit

pressure and based on the isentropic conditions we calculated the thermodynamic parameters of these nozzle exit state points (e_o,e",...). On the isentropic line $c_o t_o e_o e"$, only certain points have given parametric values such as pressure ratio p_c/p, pressure p, temperature T, enthalpic value H, molecular weight M, specific heat at constant pressure c_p etc. and the values of partial derivatives $\left(\frac{\partial \ln M}{\partial \ln p}\right)_T$ and $\left(\frac{\partial \ln M}{\partial \ln T}\right)_p$ (see references 1 and 4 for the calculation formulas and methods for these two partial derivatives). Therefore, this isentropic line can act as the reference line for extrapolution calculations. A typical isentropic reference line is listed in Table 1. The parameters on the top half of the table were taken from Reference 5.

(1) 参 数	(2)												
p_s/p	1	1.737	10	40.027	60.046	100	200	400	600	800	1000	1200	10000
(5) ρ, 油开/混合气(油相)	60.69	39.48	6.069	1.667	1	0.6089	0.2268	0.1701	0.1154	0.0851	0.0686	0.0227	0.0068
T, K	3600	3386	3015	2674	2536	2409	2218	2151	2075	1981	1898	1698	1445
(6) H, 大中/油开	0	−249.9	−942.0	−1412.1	−1666.2	−1676.9	−1968.2	−2038.7	−2133.9	−2198.6	−2247.1	−2464.9	−2661.7
(7) M,油开/油开混合	19.732	19.974	16.696	17.140	17.310	17.423	17.702	17.761	17.814	17.878	17.907	17.992	18.014
(8) c_p, 大中/油开 K	2.9081	2.9481	2.3704	1.9866	1.7388	1.6279	1.2694	1.1787	1.0977	0.9784	0.9217	0.7157	0.6136
$\left(\frac{\partial \ln M}{\partial \ln p}\right)_T$	0.00000	0.04589	0.02958	0.01944	0.01484	0.01234	0.00611	0.00408	0.00198	0.00270	0.00212	0.00046	0.00004
$\left(\frac{\partial \ln M}{\partial \ln T}\right)_p$	−0.0458	−0.0804	−0.0116	−0.4988	−0.3638	−0.5125	−0.1786	−0.1479	−0.1098	−0.0849	−0.0686	−0.0172	−0.0018
$D_T = \left(\frac{\partial \ln T}{\partial \ln p}\right)_H$	0.04128	0.03888	0.03215	0.02619	0.02300	0.02190	0.01579	0.01404	0.01148	0.00969	0.00835	0.00267	0.00072
$D_H = \left(\frac{\partial \ln M}{\partial \ln p}\right)_T$	0.01523	0.01384	0.00991	0.00716	0.00520	0.00550	0.00351	0.00308	0.00233	0.00180	0.00153	0.00041	0.00004
$\theta_T = \left(\frac{\Delta T}{\Delta \ln p}\right)_s$	357°	318.4	279.6	242.4	230.9	226.0	220.4	232.9	256.8	265.8	265.2	255.2	253.0
$\theta_H = \left(\frac{\Delta H}{\Delta \ln p}\right)_s$	−0.434°	−0.4062	−0.2804	−0.3498	−0.3178	−0.2956	−0.2539	−0.2851	−0.1888	−0.1533	−0.1293	−0.0775	−0.0161
$\theta_M = \left(\frac{\Delta M}{\Delta \ln p}\right)_s$	304°	430.8	396.4	334.2	301.9	287.6	265.1	245.1	234.8	229.4	216.2	190.5	164.9
$\theta_{DT} = \left(\frac{\Delta D_T}{\Delta \ln p}\right)_s$	0.0330°	0.0307[illegible]	0.0250[illegible]	0.0242[illegible]	0.0246[illegible]	0.0249[illegible]	0.0225[illegible]	0.0208[illegible]	0.0163[illegible]	0.0137[illegible]	0.0101[illegible]	0.0050[illegible]	0.001[illegible]
$\theta_{DH} = \left(\frac{\Delta D_H}{\Delta \ln p}\right)_s$	0.0220°	0.0225[illegible]	0.0222[illegible]	0.0219[illegible]	0.0218[illegible]	0.0218[illegible]	0.0218[illegible]	0.0217[illegible]	0.0216[illegible]	0.0215[illegible]	0.0214[illegible]	0.0210[illegible]	0.0207

(9) • 外插得到的数据

Table 1. (see next page)

Table 1 Parameters on the isentropic reference line (gaseous hydrogen and gaseous oxygen propellant, mixing ratio O/F=7.9365, initial enthalpic value H_{CO}=O major calories/kg).

Key: (1) Parameter; (2) Conbustion chamber; (3) Throat; (4) Nozzle exit; (5) Kg/cm^2 (absolute; (6) Major calories/kg; (7) Kg/kg mol; (8) Major calories/kg; (9) Data obtained by extrapolation.

On the isentropic reference line, the thermodynamic parameters of each point outside the known parametric points can approximately be calculated by the following interpolation formulas:

$$\left.\begin{aligned} F &= Q\ln\rho \\ (\Delta F)_i &= Q(\Delta\ln\rho)_i \end{aligned}\right\} \qquad (1)$$

In the formulas, F indicates the T,H,M... etc. parameters; Q is the interpolation coefficient and is determined based on the parameters of the two adjacent known points.

For the isentropic reference line in Table 1, the calculation results of Q_T, Q_M and Q_H etc. interpolation coefficients are listed in the lower half of the table.

III. Isenthalpic Partial Derivatives and Isenthalpic Relational Formula

Based on the related formulas in References 4 and 5, the two isenthalpic partial derivatives used in this paper can be indicated by the following formulas:

$$D_T = \left(\frac{\partial\ln T}{\partial\ln\rho}\right)_H = \frac{-R}{c_p M}\left(\frac{\partial\ln M}{\partial\ln T}\right)_\rho \qquad (2)$$

$$D_H = \left(\frac{\partial\ln M}{\partial\ln\rho}\right)_H = \frac{-R}{c_p M}\left(\frac{\partial\ln M}{\partial\ln T}\right)_\rho^2 + \left(\frac{\partial\ln M}{\partial\ln\rho}\right)_T \qquad (3)$$

In the formulas, R is the commonly used gas constant (1.98726 major calories/kg mol K).

For the isentropic reference line in Table 1, the D_T, D_M, Q_{DT} and Q_{DM} values calculated by each of the above formulas are listed in the lower half of the table.

The relational formula of the temperature and molecular weight on the isenthalpic line is

$$(\Delta \ln T)_H = D_T(\Delta \ln \rho)_H \qquad (4)$$

$$(\Delta \ln M)_H = D_M(\Delta \ln \rho)_H \qquad (5)$$

We substituted the first law of thermodynamics expression and the state equation into the differential formula of entropy and obtained

$$ds = \frac{dH}{T} - \frac{R}{M}\frac{dp}{p}$$

As regards isenthalpic line (dH=0), from this formula we obtained

$$(\Delta s)_H = -\frac{R}{M}(\Delta \ln \rho)_H \qquad (6)$$

IV. Establishment of the Extrapolation Formulas

1. Formulas of the Combustion Chamber's Thermodynamic Parameters and the Characteristic Velocity

When the propellant's initial enthalpic value $H_c=H_{co}$ and the combustion chamber pressure $p_c \neq p_{co}$, based on $\Delta H_c=H_c-H_o$ and the known data of the c_o point, we can calculate the parameters of the c' point in Fig. 1 from formula (1). Afterwards, based on the parameters of the c' point and $p=p_c$, we can calculate the parameters of the c point from formulas (4) and (5). As a result, we obtained the combustion chamber temperature and molecular weight formulas

$$T_c = \left(T_{co} + \frac{Q_T \Delta H_c}{Q_H}\right) \exp\left[\left(D_{Tco} + \frac{Q_{DT}\Delta H_c}{Q_H}\right)\left(\ln\frac{p_c}{p_{co}} - \frac{\Delta H_c}{Q_H}\right)\right] \quad (7)$$

$$M_c = \left(M_{co} + \frac{Q_M \Delta H_c}{Q_H}\right) \exp\left[\left(D_{Mco} + \frac{Q_{DM}\Delta H_c}{Q_H}\right)\left(\ln\frac{p_c}{p_{co}} - \frac{\Delta H_c}{Q_H}\right)\right] \quad (8)$$

Because the characteristic velocity c* is in direct ratio to $\sqrt{T_c/M_c}$, the extrapolation formula of the characteristic velocity can be written as

$$c^* = c_0^* \sqrt{T_c M_{co}/M_c T_{co}} \quad (9)$$

2. Formulas of the Nozzle Exit's ($p=p_c$) Thermo amic Parameters

We should use formula (6) between points c and c and points e and e':

$$\ln\frac{p_{c'}}{p_c} = \frac{M_{c'}}{M_{e'}}\ln\frac{p_{e'}}{p_e}$$

When we substitute formula (1) into this formula, we obtain

$$\ln\frac{p_{c'}}{p_{co}} = \ln\frac{p_c}{p_{co}} + \frac{M_{co}\left(\frac{\Delta H_c}{Q_H} - \ln\frac{p_c}{p_{co}}\right)}{M_{co} + \frac{Q_M \Delta H_c}{Q_H}} \quad (10)$$

In the formula, M_{eo} is the approximate value of M_e, and it is a known molecular weight of the $p=p_{ep}$ point close to p_c, on the isentropic reference line. In order to select p_{eo} and determine M_{eo}, we can calculate the initial value of p_c, according to the following formula:

$$p_{c'(1)} = p_c \exp\left[\frac{M_{c'}}{M_{co}}\left(\frac{\Delta H_c}{Q_H} - \ln\frac{p_c}{p_{co}}\right)\right] \quad (11)$$

Key: (1) Initial.

This formula was approximately obtained from formula (10). The $M_{e'}$ in the formula is the known molecular weight of the

isentropic reference line's lowest point.

Interpolation coefficients Q_T, Q_{DT}, Q_M, Q_{DM} and Q_H in formulas (7), (8), (10) and (11) use the numerical value close to p_{co}. When $\Delta H_c < 0$, we use the mean value of c_o-t_o; when $\Delta H_c > 0$, we use the numerical value of $p > p_{co}$.

Based on the known data of the e_o point and the $\frac{p_{c'}}{p_{co}}$ value calculated from formula (10), we can calculate the parameters of e' from formula (1). Afterwards, based on the parameters of the e' point and $p=p_c$, we can calculate the parameters of the e point from formulas (4) and (5). As a result, we obtain the formulas of the nozzle exit's temperature and molecular weight

$$T_e = \left(T_{co} + Q_T \ln \frac{p_{c'}}{p_{co}}\right) \exp\left[\left(D_{Tco} + Q_{DT} \ln \frac{p_{c'}}{p_{co}}\right)\left(\ln \frac{p_e}{p_{co}} - \ln \frac{p_{c'}}{p_{co}}\right)\right] \quad (12)$$

$$M_e = \left(M_{co} + Q_M \ln \frac{p_{c'}}{p_{co}}\right) \exp\left[\left(D_{Mco} + Q_{DM} \ln \frac{p_{c'}}{p_{co}}\right)\left(\ln \frac{p_e}{p_{co}} - \ln \frac{p_{c'}}{p_{co}}\right)\right] \quad (13)$$

3. Formulas of the Specific Thrust and Other Parameters

When we substitute $H_c=H_{c'}=H_{co}+\Delta H_c$ and $H_e=H_{e'}=H_{eo}+Q_H \ln \frac{p_{c'}}{p_{co}}$ into design altitude specific thrust formula $I=294.98\sqrt{(H_c-H_e)/1,000}$, we obtained

$$I = 9.328\sqrt{H_{co} + \Delta H_c - H_{eo} - Q_H \ln \frac{p_{c'}}{p_{co}}} \quad (14)$$

Interpolation coefficients Q_T, Q_{DT}, Q_M, Q_{DM} and Q_H in formulas (12) to (14) use numerical values close to p_{co}. When $\ln \frac{p_{c'}}{p_{co}} < 0$, we use a numerical value smaller than p_{co}; when $\frac{p_{c'}}{p_{co}} > 0$, we use a numerical value larger than p_{co}.

The nozzle exit's specific area and the nozzle's area ratio can be calculated by the following formula:

$$I_s = 86.50\,T_c/(p_c M_c) \quad (15)$$

$$\varepsilon = I_{sg} p_c / c^* \quad (16)$$

V. Accuracy of the Extrapolation Formulas

Based on the above formulas, we can carry out extrapolation calculations. The extrapolation calculation results of the hydrogen and oxygen propellant with a mixing ratio of O/F=7.9365, nozzle area ratio, characteristic velocity, combustion chamber temperature and designed altitude specific thrust are listed in Table 2, 3 and 4 and Fib. 2. In order to make comparisons, the corresponding precise calculation results [5,6] and the extrapolation calculation results of Reference 5 are also listed in the tables and figure.

p_c/p	(1)液氧液氢，焓值 $H_c=-190.6$ 大卡/公斤			(5)气氢气氧，焓值 $H_c=629.1$ 大卡/公斤		
	(2)精确值	(3)本文的外推值	文献5的外推值(4)	(6)精确值	(7)本文的外推值	文献5的外推值(8)
10	2.468	2.476	2.289	2.466	2.459	2.337
40.83	7.151	7.188	7.130	7.169	7.196	7.279
68.05	10.75	10.80	10.77	10.81	10.77	11.00
100	14.69	14.74	14.70	14.81	14.70	15.01
300	36.28	36.40	35.70	37.02	37.05	36.45
400	46.04	46.19	45.04	47.22	47.29	45.98
600	64.44	64.58	62.49	66.66	66.55	63.80
800	81.77	81.90	78.83	85.21	84.97	80.49
1000	98.31	98.41	94.40	103.2	103.6	96.38

Table 2 Comparison of nozzle area ratio calculated by extrapolation and the precise values (hydrogen and oxygen propellant, mixing ratio O/F=7.9365, combustion chamber pressure p_c=6.805kg/cm^2, absolute).

Key: (1) Liquid oxygen and liquid hydrogen, enthalpic value H_c=-190.6 major calories/kg; (2) Precise value; (3) Extrapolation value of this paper; (4) Extrapolation value of Reference 5; (5) Gaseous hydrogen and gaseous oxygen enthalpic value H_c=629.1 major calories/kg; (6) Precise value; (7) Extrapolation value of this paper; (8) Extrapolation value of Reference 5.

(1) 燃烧室压力 p_c 公斤/厘米², 绝对	(2) 气氢气氧, 焓值 $H_c=0$ 大卡/公斤			(7) 液氢液氧, 焓值 $H_c=-190.6$ 大卡/公斤			(12) 气氢气氧, 焓值 $H_c=629.1$ 大卡/公斤		
	(3) 精确值	(4) 外推值 (5) 本文	(6) 文献5	(8) 精确值	(9) 外推值 (10) 本文	(11) 文献5	(13) 精确值	(14) 外推值 (15) 本文	(16) 文献5
68.05	2197	2197	2197	2156	2156	2157	2324	2326	2329
40.83	2184	2182	2184	2144	2142	2144	2308	2310	2316
6.805	2136	2132	2139	2099	2094	2099	2251	2254	2271

(17) 注: 表中特征速度数值的单位是米/秒

Table 3 Comparison of characteristic velocity calculated by extrapolation and the precise values (hydrogen and oxygen propellant, mixing ratio O/F=7.9365).

Key: (1) Combustion chamber pressure p_C, kg/cm^2, absolute; (2) Gaseous hydrogen and gaseous oxygen propellant, enthalpic value H_C=0 major calories/kg; (3) Precise value; (4) Extrapolation value; (5) This paper; (6) Reference 5; (7) Liquid hydrogen and liquid oxygen, enthalpic value H_C=-190.6 major calories/kg; (8) Precise value; (9) Extrapolation value; (10) This paper; (11) Reference 5; (12) Gaseous hydrogen and gaseous oxygen, enthalpic value H_C=629.1 major calories/kg; (13) Preciate value; (14) Extrapolation value; (15) This paper; (16) Reference 5; (17) Note: in the table, the unit of the characteristic velocity is meters/second.

(1) 燃烧室压力 p_c 公斤/厘米², 绝对	1.02	2.04	4.08	10.21	20.42	40.83	61.25	81.56
(2) 精确值	3039	3127	3217	3341	3437	3534	3591	3632
(3) 本文的外推值	3053	3138	3225	3344	3437	3533	3590	3631

(4) 注: 表中燃烧室温度数值的单位是K

Table 4 Comparison of combustion chamber pressure temperature calculated by extrapolation and the precise values (liquid hydrogen and liquid oxygen propellant, mixing ratio O/F=7.9365).

Key: (1) Combustion chamber pressure p_C, kg/cm^2, absolute; (2) Precise value; (3) Extrapolation value of this paper; (4) Note: in this table, the unit of the combustion chamber temperature numerical value is K.

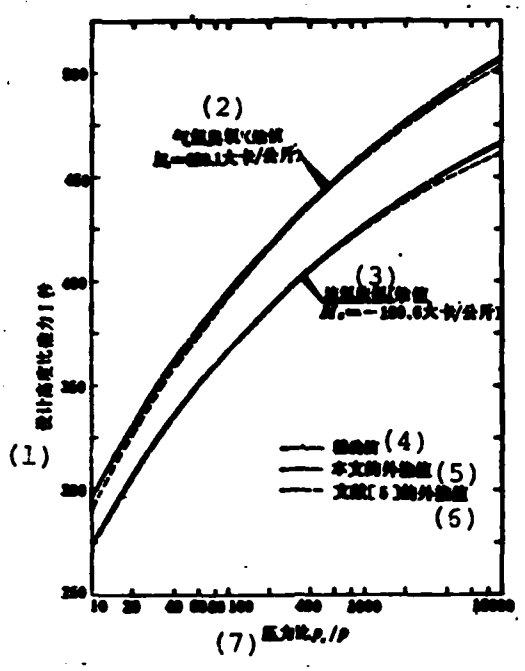

Fig. 2 Comparison of design altitude specific thrust calculated by extrapolation and the precise values (hydrogen and oxygen propellant, mixing ratio O/F=7.9365, combustion chamber pressure p_c=6.805 kg/cm^2, absolute).

Key: (1) Design altitude specific thrust I seconds; (2) Gaseous hudrogen and gaseous oxygen (enthalpy value H_c=629.1 major calories/kg); (3) Liquid hydrogen and liquid oxygen (enthalpy value H_c=-190.6 major calories;kg); (4) Precise value; (5) Extrapolution value of this paper; (6) Extrapolation value of Reference 5. (7) Pressure ratio p_c/p.

We can see from Tables 2 to 4 and Fig. 2 that the precision of the extrapolation formulas in this paper are relatively high and can be suitably used for the extrapolation calculations of the real parametric ranges of rocket engines.

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THERMODYNAMIC CALCULATION OF THE SYMBOLIC FORMULA FOR ROCKET ENGINES

Fang Zhaokui

Abstract

A symbolic element is substituted for chemical elements which cause practical chemical reaction. With the use of the symbolic formula, a new calculation method has been set up to calculate theoretical performance of the propellant. It will be able to devise a general computer program for chemical equilibrium of rocket engines which does not depend on practical chemical elements.

In the past, China widely used a type of chemical thermodynamic calculation. Its major feature was that the chemical reaction formula must be linked with the concrete chemical elements of the propellant. This made it difficult to design general programs. The thermodynamic calculation of the symbolic formula proposed in this paper eliminates the above mentioned difficulties.

I. Symbolic Elements and Their Molecular Formula

We give a pair of positive integers i and j, define a set of symbolic elements A_j for any propellants with j type elements and which produce i type combustion products as well as their corresponding symbolic element atomic number a_j. We use the ordered permutation of symbolic element A_j:

$$\prod_{\mu=1}^{i} A_{\beta_\mu} = A_{\beta_1} A_{\beta_2} A_{\beta_3} \cdots A_{\beta_i} \quad (i = 1, 2, \cdots i) \qquad (1)$$

It indicates the i type combustion product molecular formula produced after propellant combustion. Symbol $\prod$ indicates the ordered permutation as shown in formula (1).

For example, we use the symbolic elements A_1, A_2, A_3, A_4 to replace the four element propellant of C, H, O, N and let the i type combustion product be C O. Naturally, based on the definition, its symbolic element molecular formula is:

$$CO - \prod^{i} A_{j a_{ji}} - A_1 A_2 A_3 A_4 \qquad (2)$$

The connection of the i and j naming sequence with the product and element is arbitrary, yet as soon as we gave the relationship formula (2) solely determined the CO.

II. Chemical Equilibrium Equation of the Symbolic Element Combustion Product

Definition: for any molecular type combustion product $\prod^{j} A_j a_{ji}$, we let its dissociation reaction combine with symbolic element A_j:

$$\prod^{j} A_{j a_{ji}} \longrightarrow \sum^{j} a_{ji} A_j \quad (i = 1, 2 \cdots i) \qquad (3)$$

It acts as the chemical equilibrium reaction formula. Because it is invested with the symbolic element effective partial meaning, it coincides with the laws of conventional multiplication:

$$a_{ji} \times A_j = \begin{cases} 0 & \text{(1) 若 } a_{ji} = 0 \\ a_{ji} A_j & \text{(2) 若 } a_{ji} \neq 0 \end{cases} \qquad (4)$$

Key: (1) If; (2) If.

From the chemical equilibrium reaction theory, the chemical equilibrium equation corresponding to formula (3) is:

$$P_{\prod^{j} A_{j a_{ji}}} \Big/ \left(P_{A_1}^{a_{j1}} \times P_{A_2}^{a_{j2}} \times \cdots \times P_{A_j}^{a_{ji}} \right) = f_i(T) \quad (i = 1, 2 \cdots i) \qquad (5)$$

In the formula, $P_{\prod^{j} A_{j a_{ji}}}$ P_{A_j} separately indicate the partial pressure of symbolic element molecular product $\prod^{j} A_j a_{ji}$ and

atomic product A_j in the combustion process and $f_i(T)$ is the equilibrium constant of this dissociation reaction under temperature T. If there is basically no certain element existing in this molecule (for example, basically no hydrogen content in the CO molecule), then $P^{o}_{A_j}=1$ because of the conventional mathematical law and we must be able to satisfy equation (5). We used the logarithm for formula (5):

$$\ln P_j - \ln\prod A_{ij}^{a_{ij}} = \ln f_i(T) + \sum_{j}^{J} a_{ij}\ln P_{A_j} \qquad (6)$$

By using formula (6), we can cause the molecular type partial pressure to transform into atomic type partial pressure, eliminate the molecular type variable and thus greatly reduce the number of equations.

III. The Symbolic Element Propellant Matrix and Its Normalized Process

Definition: we assume there is a complex propellant composed from the n type pure chemical substance mixture and molecular formulas of each type of pure chemical substance. The enthalpy and mixture weight percentage are separately $\prod^{j} A_{ij}, H_i, z_i \ (i=1,2,\cdots n)$ and then the characteristics of this propellant can be completely determined by the following matrix:

$$A(n, j+2) = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1j} & H_1 & z_1 \\ a_{21} & a_{22} & \cdots & a_{2j} & H_2 & z_2 \\ \vdots & \vdots & & \vdots & \vdots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nj} & H_n & z_n \end{pmatrix} \qquad (7)$$

Formula (7) is called the propellant matrix. During performance calculations, it is only n-cessary to consider the theoretical performance of the unit mass. For this reason

Definition: we take the symbolic element molecular formula

of a unit mole propellant with a molecular weight of 1 as the standardized equivalent weight formula of the propellant. The process in which it transforms from the original propellant to the symbolic element propellant equivalent formula is called the symbolic element propellant standardization process.

Theorem: we assume there is complex propellant (7), μ_j is the atomic weight of symbolic element A_j. When we let matrix

$$B(n) = \begin{pmatrix} x_1 / \sum_{j}^{j} a_{1j} a_{j0} \\ x_2 / \sum_{j}^{j} a_{2j} a_{j0} \\ \vdots \\ x_n / \sum_{j}^{j} a_{nj} a_{j0} \end{pmatrix} \qquad (8)$$

then the normalization process of propellant (7) is realized by the matrix operation of the following formula

$$A(j+1) = A'(n, j+1) \times B(n) = \begin{pmatrix} a_{10} \\ a_{20} \\ \vdots \\ a_{n0} \\ H_0 \end{pmatrix} \qquad (9)$$

In the formula, A'(n,j+1) is the transposed matrix of matrix A(n,j+1) obtained after deleting the last column in matrix (7). After normalization of (9) there is a column matrix. The lower symbol "0" of column matrix element a_{j0} indicates that it does not belong in combustion product number "i". From (9) we can deduce

$$\sum_{j}^{j} a_{ij} a_{j0} = 1 \qquad (10)$$

This is the inevitable result of standardization processing. For double element liquid propellants, if the combusting agent of corresponding formulas (7) and (8) is A(n,j+2), B(n), the oxidizing agent is A(m,j+2), B(m) and K is the mixing ratio,

then the standardization process of this type of complex double element propellant is:

$$A(j+1) = [A'(n, j+1) \times B(n) + KA'(m, j+1) \times B(m)]/(1+K) \quad (11)$$

Finally, we obtained a column matrix in the same way. The proof of (9), (10) and (11) is deleted.

IV. Basic Equations of the Thermodynamic Calculation of the Symbolic Formula and the Program Design

Assuming the propellant is determined by positive integers i and j and normalized matrix A(j+1), then the combustion reaction standard formula is:

$$M \prod^{j} A_{\mu\beta_\mu} \longrightarrow \sum^{i} P_i \prod^{j} A_{\mu\beta_\mu} \quad (12)$$

The above formula shows that when the M mol propellant combusts, it separately produces combustion product $\prod^{j} A_u a_{ji}$ with partial pressure P_i, yet when there is a condensed phase, P_i should be viewed as the molar number of the condensed phase product. Now, the four basic equations of the thermodynamic calculations of the symbolic formula can be rewritten as:

1. Conservation of mass equation:

$$a_\beta = \sum^{i} a_{\mu\beta} P_i / M \quad j = 1, 2, \cdots j \quad (13)$$

2. Conservation of energy equation:

$$\left.\begin{aligned} H_0 &= \sum^{i} (H_T^\circ)_i P_i / M \quad \text{(等焓-燃烧室状态)} \\ S_0 &= \sum^{i} [(S^\circ)_i - \beta_i] P_i / M \quad \text{(等熵-喷管状态)} \end{aligned}\right\} \begin{matrix} (1) \\ (2) \end{matrix} \quad (14)$$

Key: (1) Isenthalpy-combustion chamber condition;
(2) Inentropy-nozzle condition.

3. Chemical equilibrium equation:

$$(F_T^\circ)_i/(RT) + \ln\omega_i - \sum^{j} a_{ij}[(F_T^\circ)_j/(RT) + \ln\omega_j] = 0 \quad i = 1, 2, \cdots i, \qquad (15)$$

In formulas (14) and (15), $(H_T^\circ)_i$, $(S_T^\circ)_i$ and $(F_T^\circ)_i$ are separately the enthalpy, entropy and free energy when the i type product is in temperature T.

$$\beta_i = \begin{cases} R\ln P_i & \text{(对于气相) (1)} \\ 0 & \text{(对于凝聚相) (2)} \end{cases} \qquad \omega_i = \begin{cases} P_i & \text{(对于气相) (3)} \\ 1 & \text{(对于凝聚相) (4)} \end{cases}$$

Key: (1) For the gas phase; (2) For the condensed phase; (3) For the gaseous phase; (4) For the condensed phase.

R is a molar common suitable constant. The differentiating formula of the solidifying phase is deleted.

4. Dalton's law:

$$P_0 = \sum^{i} P_i \quad \text{(仅对气相) (1)} \qquad (16)$$

Key: (1) Only for the gaseous phase.

Solving the above mentioned equations when A(n,j+2), A(m,j+2), K, P_o, H_o and μ_j are known forms the basic proposition of the thermodynamic calculations.

In the program design, we must linearize the group of equations, use (6) to reduce the number of equations and use the partial derivative approximation and convergence factor to solve the problem of the arbitrariness of the initial value in a large range. We used BCY language to draw up the commonly used program for the thermodynamic calculation of the symbolic formula and the calculations carried out on a 109C computer for several tens of propellants were all successful. The above contents were limited by space and we will not go into further detail.

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